

chain nodes :

10 11 15 16 17 18 19 26 27 28 29 30 31 32 36 37 38 39 40 43

ring nodes :

1 2 3 4 5 6 7 8 9

chain bonds :

7-26 9-10 10-11 27-43 28-43 29-30 29-31 31-32 36-37 36-38 39-40

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9

exact/norm bonds :

6-9 7-26 8-9 27-43 28-43 29-30 36-37 36-38 39-40

exact bonds :

5-7 7-8 9-10 10-11 29-31 31-32

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 :

G1:[*1],[*2],[*3],[*4],[*5]

G2:[*6],[*7],[*8],[*9]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:Atom
 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS
 30:CLASS 31:CLASS 32:CLASS 36:CLASS 37:CLASS 38:CLASS 39:CLASS 40:CLASS 43:CLASS

* * * * * Welcome to STN International * * * * *

| | | |
|---------------------|---------|---|
| <u>NEWS 1</u> | | Web Page URLs for STN Seminar Schedule - N. America |
| <u>NEWS 2</u> | | "Ask CAS" for self-help around the clock |
| <u>NEWS 3</u> | Feb 24 | PCTGEN now available on STN |
| <u>NEWS 4</u> | Feb 24 | TEMA now available on STN |
| <u>NEWS 5</u> | Feb 26 | NTIS now allows simultaneous left and right truncation |
| <u>NEWS 6</u> | Feb 26 | PCTFULL now contains images |
| <u>NEWS 7</u> | Mar 04 | SDI PACKAGE for monthly delivery of multifile SDI results |
| <u>NEWS 8</u> | Mar 24 | PATDPAFULL now available on STN |
| <u>NEWS 9</u> | Mar 24 | Additional information for trade-named substances without structures available in REGISTRY |
| <u>NEWS 10</u> | Apr 11 | Display formats in DGENE enhanced |
| <u>NEWS 11</u> | Apr 14 | MEDLINE Reload |
| <u>NEWS 12</u> | Apr 17 | Polymer searching in REGISTRY enhanced |
| <u>NEWS 13</u> | Jun 13 | Indexing from 1947 to 1956 added to records in CA/CAPLUS |
| <u>NEWS 14</u> | Apr 21 | New current-awareness alert (SDI) frequency in WPIDS/WPINDEX/WPIX |
| <u>NEWS 15</u> | Apr 28 | RDISCLOSURE now available on STN |
| <u>NEWS 16</u> | May 05 | Pharmacokinetic information and systematic chemical names added to PHAR |
| <u>NEWS 17</u> | May 15 | MEDLINE file segment of TOXCENTER reloaded |
| <u>NEWS 18</u> | May 15 | Supporter information for ENCOMPPAT and ENCOMPLIT updated |
| <u>NEWS 19</u> | May 19 | Simultaneous left and right truncation added to WSCA |
| <u>NEWS 20</u> | May 19 | RAPRA enhanced with new search field, simultaneous left and right truncation |
| <u>NEWS 21</u> | Jun 06 | Simultaneous left and right truncation added to CBNB |
| <u>NEWS 22</u> | Jun 06 | PASCAL enhanced with additional data |
| <u>NEWS 23</u> | Jun 20 | 2003 edition of the FSTA Thesaurus is now available |
| <u>NEWS 24</u> | Jun 25 | HSDB has been reloaded |
| <u>NEWS 25</u> | Jul 16 | Data from 1960-1976 added to RDISCLOSURE |
| <u>NEWS 26</u> | Jul 21 | Identification of STN records implemented |
| <u>NEWS 27</u> | Jul 21 | Polymer class term count added to REGISTRY |
| <u>NEWS 28</u> | Jul 22 | INPADOC: Basic index (/BI) enhanced; Simultaneous Left and Right Truncation available |
| <u>NEWS 29</u> | AUG 05 | New pricing for EUROPATFULL and PCTFULL effective August 1, 2003 |
| <u>NEWS EXPRESS</u> | April 4 | CURRENT WINDOWS VERSION IS V6.01a, CURRENT MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP), AND CURRENT DISCOVER FILE IS DATED 01 APRIL 2003 |
| <u>NEWS HOURS</u> | | STN Operating Hours Plus Help Desk Availability |
| <u>NEWS INTER</u> | | General Internet Information |
| <u>NEWS LOGIN</u> | | Welcome Banner and News Items |
| <u>NEWS PHONE</u> | | Direct Dial and Telecommunication Network Access to STN |
| <u>NEWS WWW</u> | | CAS World Wide Web Site (general information) |

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 13:48:22 ON 07 AUG 2003

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 13:48:30 ON 07 AUG 2003

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 6 AUG 2003 HIGHEST RN 562043-52-1

DICTIONARY FILE UPDATES: 6 AUG 2003 HIGHEST RN 562043-52-1

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See [HELP CROSSOVER](#) for details.

Experimental and calculated property data are now available. See [HELP PROPERTIES](#) for more information. See STN Note 27, Searching Properties in the CAS Registry File, for complete details:

<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=>

L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1 STR

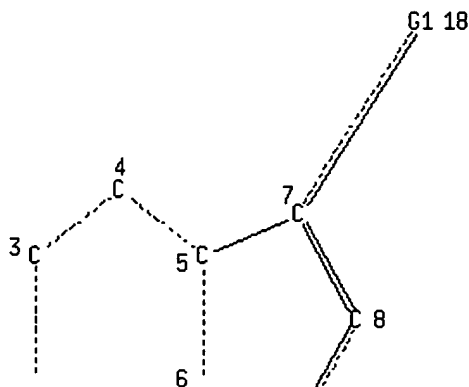
C 16

S 14

N 15

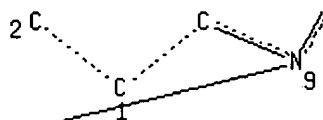
O 13

19
O
||
S 17
||
O
20



Page 1-B

G20
12
Page 2-A



10 C M2

Cb 11

Page 2-B

1

Page 2-C

VAR G1=13/14/15/16/17

REP G20=(1-2) 10-9 10-11

NODE ATTRIBUTES:

| | | | |
|--------|-------|----|----|
| HCOUNT | IS M2 | AT | 10 |
| NSPEC | IS R | AT | 1 |
| NSPEC | IS R | AT | 2 |
| NSPEC | IS R | AT | 3 |
| NSPEC | IS R | AT | 4 |
| NSPEC | IS R | AT | 5 |
| NSPEC | IS R | AT | 6 |
| NSPEC | IS R | AT | 7 |
| NSPEC | IS R | AT | 8 |
| NSPEC | IS R | AT | 9 |
| NSPEC | IS C | AT | 10 |
| NSPEC | IS C | AT | 11 |
| NSPEC | IS C | AT | 12 |
| NSPEC | IS C | AT | 13 |
| NSPEC | IS C | AT | 14 |
| NSPEC | IS C | AT | 15 |
| NSPEC | IS C | AT | 16 |
| NSPEC | IS C | AT | 17 |
| NSPEC | IS C | AT | 18 |
| NSPEC | IS C | AT | 19 |
| NSPEC | IS C | AT | 20 |

DEFAULT MLEVEL IS ATOM

MLEVEL IS CLASS AT 10 13 14 15 16 17 19 20

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC I

NUMBER OF NODES IS 20

STEREO ATTRIBUTES: NONE

=> s 11

SAMPLE SEARCH INITIATED 13:49:22 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 9405 TO ITERATE

10.6% PROCESSED 1000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

46 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 182292 TO 193908
PROJECTED ANSWERS: 7405 TO 9899

L2 46 SEA SSS SAM L1

=> s 11 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 147.75 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 13:49:40 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 186798 TO ITERATE

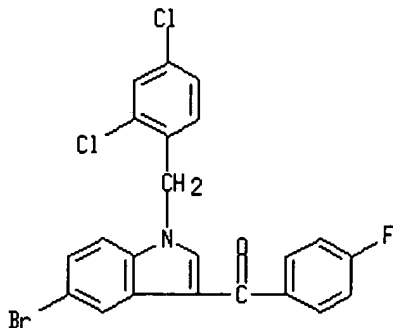
100.0% PROCESSED 186798 ITERATIONS
SEARCH TIME: 00.00.07

11659 ANSWERS

L3 11659 SEA SSS FUL L1

=> d 13

L3 ANSWER 1 OF 11659 REGISTRY COPYRIGHT 2003 ACS on STN
RN 561055-42-3 REGISTRY
CN Methanone, [5-bromo-1-[(2,4-dichlorophenyl)methyl]-1H-indol-3-yl] (4-fluorophenyl)- (9CI) (CA INDEX NAME)
MF C22 H13 Br Cl2 F N O
SR CA
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1947 TO DATE)
1 REFERENCES IN FILE CAPLUS (1947 TO DATE)

=> file hcaplus
 COST IN U.S. DOLLARS

| | SINCE FILE ENTRY | TOTAL SESSION |
|---------------------|---------------------|------------------|
| FULL ESTIMATED COST | 150.23 | 150.44 |

FILE 'HCAPLUS' ENTERED AT 13:49:55 ON 07 AUG 2003
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FILE COVERS 1907 - 7 Aug 2003 VOL 139 ISS 6
 FILE LAST UPDATED: 6 Aug 2003 (20030806/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d his

(FILE 'HOME' ENTERED AT 13:48:22 ON 07 AUG 2003)

FILE 'REGISTRY' ENTERED AT 13:48:30 ON 07 AUG 2003

L1 STRUCTURE UPLOADED
 L2 46 S L1
 L3 11659 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 13:49:55 ON 07 AUG 2003

=> s 13

L4 1557 L3

=>

L5 STRUCTURE UPLOADED

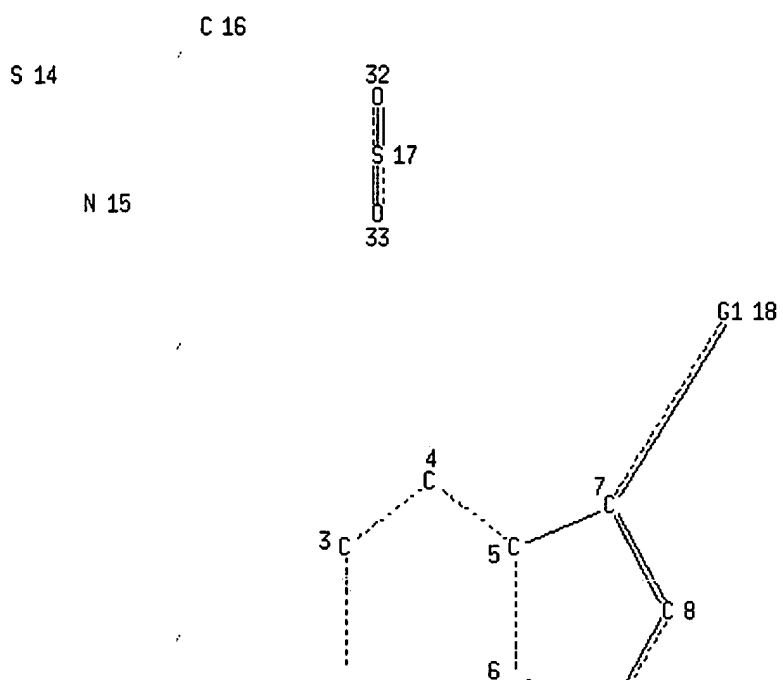
=> d 15

L5 HAS NO ANSWERS

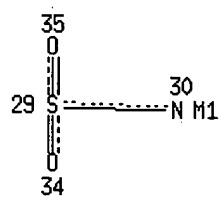
L5 STR

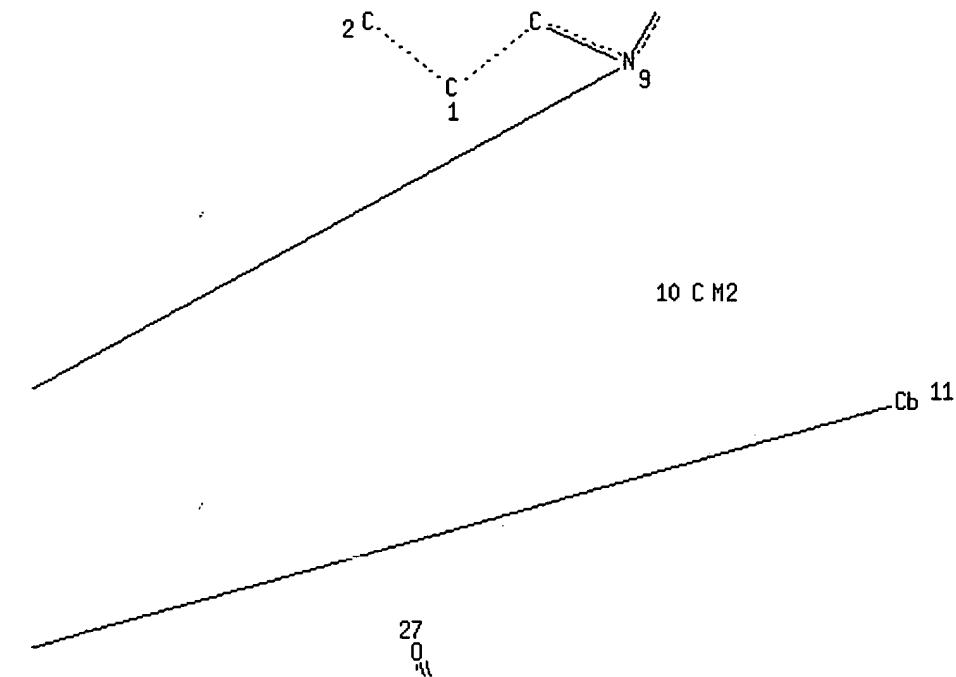
0 13

Page 1-A

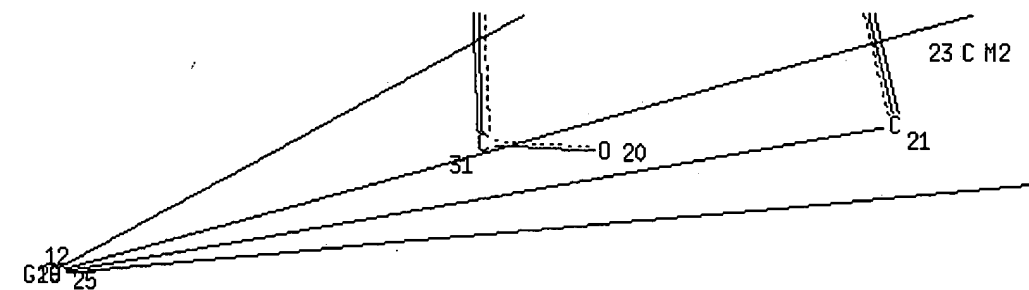


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Page 3-A



Page 3-B

```
VAR G1=13/14/15/16/17
REP G19=(1-2) 23-21 23-24
REP G20=(1-2) 10-9 10-11
NODE ATTRIBUTES:
HCOUNT IS M2 AT 10
HCOUNT IS M2 AT 23
HCOUNT IS M1 AT 24
HCOUNT IS M1 AT 28
HCOUNT IS M1 AT 30
NSPEC IS R AT 1
NSPEC IS R AT 2
NSPEC IS R AT 3
NSPEC IS R AT 4
NSPEC IS R AT 5
NSPEC IS R AT 6
```



```

NSPEC  IS R      AT   7
NSPEC  IS R      AT   8
NSPEC  IS R      AT   9
NSPEC  IS C      AT  10
NSPEC  IS C      AT  11
NSPEC  IS C      AT  12
NSPEC  IS C      AT  13
NSPEC  IS C      AT  14
NSPEC  IS C      AT  15
NSPEC  IS C      AT  16
NSPEC  IS C      AT  17
NSPEC  IS C      AT  18
NSPEC  IS C      AT  19
NSPEC  IS C      AT  20
NSPEC  IS C      AT  21
NSPEC  IS C      AT  22
NSPEC  IS C      AT  23
NSPEC  IS C      AT  24
NSPEC  IS C      AT  25
NSPEC  IS C      AT  26
NSPEC  IS C      AT  27
NSPEC  IS C      AT  28
NSPEC  IS C      AT  29
NSPEC  IS C      AT  30
NSPEC  IS C      AT  31
NSPEC  IS C      AT  32
NSPEC  IS C      AT  33
NSPEC  IS C      AT  34
NSPEC  IS C      AT  35
DEFAULT MLEVEL IS ATOM
MLEVEL  IS CLASS AT  10 13 14 15 16 17 19 20 21 22 23 24 26 27 28 29 30
        31 32 33 34 35
DEFAULT ECLEVEL IS LIMITED

```

GRAPH ATTRIBUTES:

RSPEC I

NUMBER OF NODES IS 35

STEREO ATTRIBUTES: NONE

=> s 15

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...

Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

SAMPLE SEARCH INITIATED 14:01:36 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 30 TO ITERATE

100.0% PROCESSED 30 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 272 TO 928
PROJECTED ANSWERS: 0 TO 0

L6 0 SEA SSS SAM L5

L7 0 L6

=> s 15 full

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 147.75 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 14:01:42 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 746 TO ITERATE

100.0% PROCESSED 746 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

L8 0 SEA SSS FUL L5

L9 0 L8

=> file reg

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|----------------------|------------------|---------------|
| FULL ESTIMATED COST | 2.25 | 346.33 |

FILE 'REGISTRY' ENTERED AT 14:01:52 ON 07 AUG 2003
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STRUCTURE FILE UPDATES: 6 AUG 2003 HIGHEST RN 562043-52-1
DICTIONARY FILE UPDATES: 6 AUG 2003 HIGHEST RN 562043-52-1

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STN Note 27, Searching Properties in the CAS Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=>

L10 STRUCTURE UPLOADED

=> d 110

L10 HAS NO ANSWERS

L10 STR

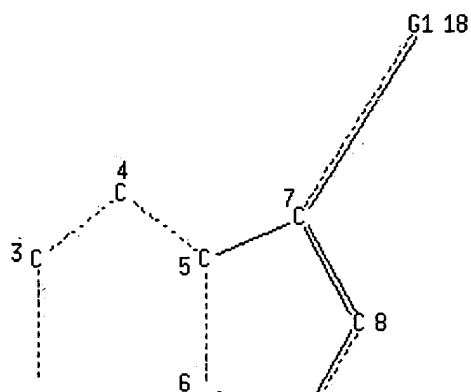
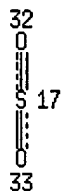
0 13

Page 1-A

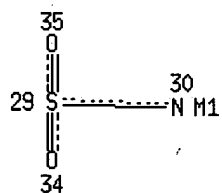
C 16

S 14

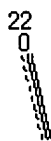
N 15

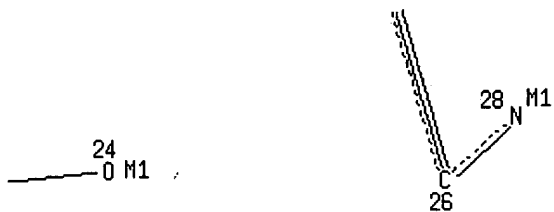
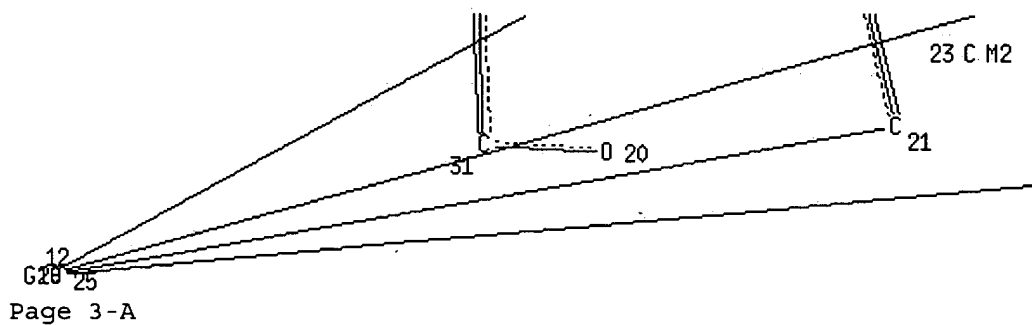
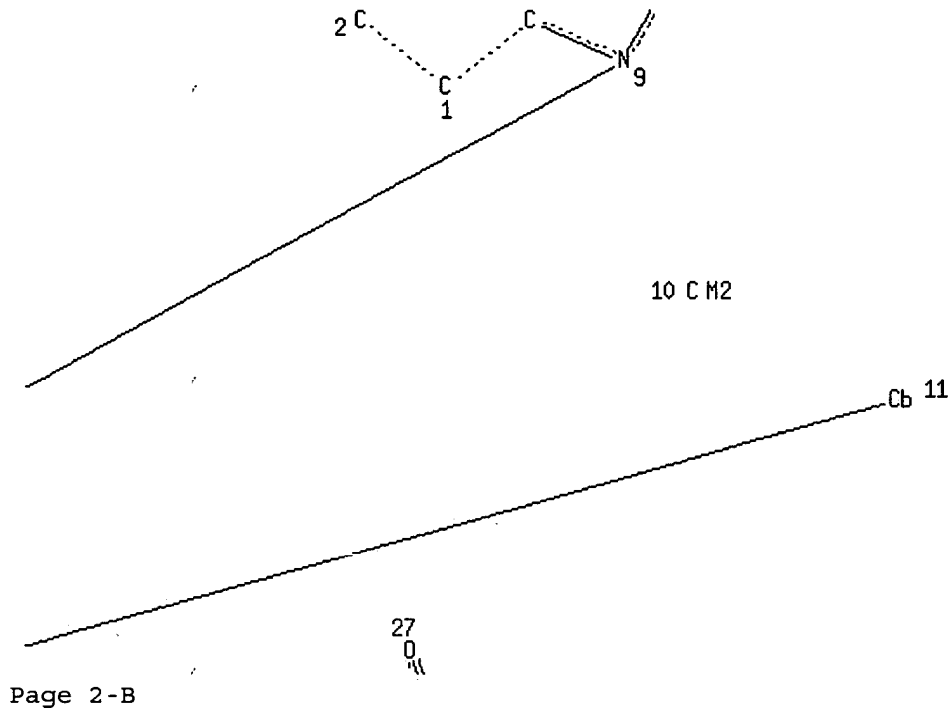


Page 1-B



Page 2-A





```

Page 3-B
VAR G1=13/14/15/16/17
REP G19=(1-2) 23-21 23-24
REP G20=(1-2) 10-9 10-11
NODE ATTRIBUTES:
HCOUNT IS M2 AT 10
HCOUNT IS M2 AT 23
HCOUNT IS M1 AT 24
HCOUNT IS M1 AT 28
HCOUNT IS M1 AT 30
NSPEC IS R AT 1
NSPEC IS R AT 2
NSPEC IS R AT 3
NSPEC IS R AT 4
NSPEC IS R AT 5
NSPEC IS R AT 6

```

```

NSPEC  IS R      AT   7
NSPEC  IS R      AT   8
NSPEC  IS R      AT   9
NSPEC  IS C      AT  10
NSPEC  IS C      AT  11
NSPEC  IS C      AT  12
NSPEC  IS C      AT  13
NSPEC  IS C      AT  14
NSPEC  IS C      AT  15
NSPEC  IS C      AT  16
NSPEC  IS C      AT  17
NSPEC  IS C      AT  18
NSPEC  IS C      AT  19
NSPEC  IS C      AT  20
NSPEC  IS C      AT  21
NSPEC  IS C      AT  22
NSPEC  IS C      AT  23
NSPEC  IS C      AT  24
NSPEC  IS C      AT  25
NSPEC  IS C      AT  26
NSPEC  IS C      AT  27
NSPEC  IS C      AT  28
NSPEC  IS C      AT  29
NSPEC  IS C      AT  30
NSPEC  IS C      AT  31
NSPEC  IS C      AT  32
NSPEC  IS C      AT  33
NSPEC  IS C      AT  34
NSPEC  IS C      AT  35
DEFAULT MLEVEL IS ATOM
MLEVEL  IS CLASS AT  10 13 14 15 16 17 19 20 21 22 23 24 26 27 28 29 30
        31 32 33 34 35
DEFAULT ECLEVEL IS LIMITED

```

GRAPH ATTRIBUTES:

RSPEC I

NUMBER OF NODES IS 35

STEREO ATTRIBUTES: NONE

=> s 110

SAMPLE SEARCH INITIATED 14:02:12 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 30 TO ITERATE

100.0% PROCESSED 30 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

```

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**

```

PROJECTED ITERATIONS: 272 TO 928

PROJECTED ANSWERS: 0 TO 0

L11 0 SEA SSS SAM L10

=> s 110 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 147.75 U.S. DOLLARS

DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y

FULL SEARCH INITIATED 14:02:21 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 746 TO ITERATE

100.0% PROCESSED 746 ITERATIONS
SEARCH TIME: 00.00.01

0 ANSWERS

L12 0 SEA SSS FUL L10

=> log y

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

148.15

494.48

STN INTERNATIONAL LOGOFF AT 14:02:28 ON 07 AUG 2003